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Superconductivity in cuprate oxide systems

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Abstract : Structure and some of the characteristic properties of high-T_c cuprate oxides (hole doped) are mentioned. Relevance of a single band Hubbard model and the t-J model in context to cuprate oxide systems is discussed. The RVB theory, mean field theories of the t-J model, the van Hove singularity scenario and the interlayer pair tunneling mechanism for superconductivity in cuprates are briefly outlined.

Keywords : High-T_c cuprates, t-J model, RVB theory, van Hove singularity scenario, pair-tunnelling mechanism.

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I. Introduction

The era of high-temperature superconductivity began with the discovery of superconductivity in La-Ba-Cu-O system around 30K by Bednorz and Muller [1]. Such a high value of transition temperature (T_c) in a material which is a very bad conductor came as a big surprise. The parent material La_2CuO_4 is an insulator and exhibits long-range antiferromagnetic (AF) ordering. With doping (La is substituted with Ba/Sr) the long-range AF order is destroyed, the AF transition temperature (T_N) decreases rapidly in $La_{2-x}Sr_xCuO_4$ from 240K to zero as x increases from zero to 0.03. At x $\sim$ 0.05 an insulator-to-metal transition takes place and superconductivity occurs in the vicinity of the metal-insulator (M-I) transition. The superconducting transition temperature (T_c) increases with doping, reaches a maximum around x = 0.15 and then

decreases. T_c becomes zero for x $\geq$ 0.23 [2]. Subsequent efforts in search of new high-T_c materials led to the discovery of superconductivity in $YBa_2Cu_3O_{7-\delta}$ system around 90K [3], in *Bi-Sr-Ca-Cu-O* system [4] with maximum T_c (T_c^m) around 110K (in Bi-2212 sample), in *Tl-Ba-Ca-Cu-O* system [5], with T_c^m around 125K (in Tl-2223 sample) and in *Hg-Ba-Ca-Cu-O* system [6] with T_c^m around 135K (in Hg-1223 sample). Under high pressure (150 kBar) T_c^m in $HgBa_2Ca_2Cu_3O_{8+\delta}$ system rises to 150K [7]. In table I a list of the high-T_c materials with corresponding T_c (at ambient pressure) is given.

Table 1. High-T_c cuprate oxide systems with corresponding number of CuO_2 planes (n) and transition temperatures (T_c).

System	n	*Nomenclature*	$T_c(K)$
$La_{2-x}(Ba/Sr)_xCuO_4$	1	La:214	38
$YBa_2Cu_3O_{7-\delta}$	2	Y:123	90
$Bi_2Sr_2Ca_{n-1}Cu_nO_{4+2n}$			
$n = 1$	1	Bi:2201	20
$n = 2$	2	Bi:2212	85
$n = 3$	3	Bi:2223	110
$Tl_2Ba_2Ca_{n-1}Cu_nO_{4+2n}$			
$n = 1$	1	Tl:2201	80
$n = 2$	2	Tl:2212	108
$n = 3$	3	Tl:2223	125
$Tl_1Ba_2Ca_{n-1}Cu_nO_{3+2n}$			
$n = 1$	1	Tl:1201	50
$n = 2$	2	Tl:1212	80
$n = 3$	3	Tl:1223	110
$n = 4$	4	Tl:1234	112
$Hg_1Ba_2Ca_{n-1}Cu_nO_{2+2n+x}$			
$n = 1$	1	Hg:1201	94
$n = 2$	2	Hg:1212	128
$n = 3$	3	Hg:1223	134

II. Crystal Structure

All the high-T_c cuprate oxide systems have layered structure with CuO_2 planes. The symmetry is either tetragonal or orthorhombic. The structure of

La_2CuO_4 is body-centered tetragonal (K_2NiF_4 type) and consists of layers of CuO_2 and LaO. Each Cu-ion is surrounded by six oxygen ions which form an elengated octahedron.

The structure of $YBa_2Cu_3O_{7-\delta}$ system consists of layer sequence Y-CuO_2-BaO-CuO-BaO-CuO_2-Y. Each Cu-ion in the CuO_2 plane is surrounded by five oxygen atoms (four in the plane and one in the BaO layer), which form a pyramid around the Cu-ion. In CuO layer, there are oxygen vacancies. For $\delta < 0.5$ (in $YBa_2Cu_3O_{7-\delta}$) the oxygens in CuO layers are ordered to form CuO chains, the corresponding structure is orthorhombic. For $\delta > 0.5$, the oxygen atoms are disordered and the structure is tetragonal.

The structure of $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ system is body- centered tetragonal having stacking sequence BiO-BiO-SrO-CuO_2-$(n-1)\times(Ca$-$CuO_2)$-SrO-BiO-BiO. The structure of $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$ is similar to that of $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ with TlO and BaO layers in place of BiO and SrO layers. The structure of $HgBa_2Ca_{n-1}Cu_nO_{2n+2+x}$ is tetragonal and similar to that of $TlBa_2Ca_{n-1}Cu_nO_{2n+3}$ system with HgO layers taking place of TlO layers and partial oxygen vacancies in HgO layers.

III. Common characteristics of high-T_c cuprate oxide families

The high-T_c cuprate oxide systems are very different from conventional superconductors. Some of the basic features are given below :

(*i*) *Quasi two – dimensional conducting planes* : All high-T_c cuprate oxide systems have CuO_2 planes and it is established that the conduction takes place in these planes whereas the other layers act as charge reservoirs.

(*ii*) *Strong anisotropy* : Cuprate oxide superconductors exihibit strong directional anosotropy. The resistivity along the c- direction (ρ_c) is much larger than that in the *ab* plane (ρ_{ab}). $\rho_c/\rho_{ab} \sim 10^2 - 10^3$ in $Y-123$ system and $\sim 10^5$ in $Bi-2212$ system. The high value of ρ_c indicates that the conduction takes place mainly in the *ab* plane. The temperature dependence of ρ_c and ρ_{ab} are also different. For most superconducting samples ρ_{ab} shows metallic behavior with linear variation with T whereas ρ_c exhibits semiconducting like behavior with exponential rise as the temperature is lowered. It should, however, be noted that the ratio ρ_c/ρ_{ab} decreases with increasing carrier concentration and for overdoped region both ρ_c and ρ_{ab} show metallic behavior with almost same temperature dependence [8].

(*iii*) *Linear temperature dependence of the resistivity* : The resistivity

ρ_{ab} of the high-T_c oxide samples shows a linear variation with temperature over a wide range of temperature. In conventional metals at low temperatures $\rho \propto T^5$ for electron-phonon scattering whereas $\rho \propto T^2$ for electron-electron scattering. At high temperature $\rho \propto T$ but at very high temperature there is a saturation in resistivity. But in high-T_c cuprate oxide systems a linear variation of ρ_{ab} with temperature is seen at as low temperature as 10K to as high temperature as 600K (in Bi-2201 system). This behavior is unusual as compared to conventional metals.

(*iv*) *Short coherence length* : High-T_c oxide superconductors have very short coherence length. $\xi_{ab} \sim$ 15-20 A and $\xi_c \sim$ 2-3 A whereas in conventional superconductors ξ is more than 1000 A. Such short coherence length in high-T_c materials suggests formation of local pairs.

(*v*) *Anomalous isotope effect* : Initial measurements of isotope-shift exponent (α) on high-T_c cuprates show that isotope effect is negligible. α was found to be less than 0.1 for La-214 systems and less than 0.05 for Y-123 system. These results led to the belief that phonons are not playing any significant role in the superconductivity of cuprates. Subsequent measurements on α have changed the situation. Now, it is established that in all cuprate oxides α is minimum at optimum doping when T_c is maximum. α is large for underdoped and overdoped systems when T_c is lower. For La-214 system $\alpha \sim$ 0.8 and for Y-123 system $\alpha \sim 0.5$ have been observed for properly underdoped samples [9].

(*vi*) *Value of the gap parameter and symmetry of the gap* : The ratio of the gap parameter to T_c is found to be much larger than the BCS value (3.52) in the ab-plane ($2\Delta_{ab}/k_B T_c \sim$ 5-7) while the gap along the c-direction is smaller ($2\Delta_c/k_B\ T_c \sim 3.5$). Recent measurements [10] have confirmed that the gap in the ab-plane is also anisotropic. The gap along the diagonal direction in the momentum space ($k_x = k_y$) is very small. This suggests that the symmetry of the superconducting gap is either d-wave or highly anisotropic s-wave.

(*vii*) *Absence of Hebel – Slichter peak in NMR relaxation rate* : In conventional superconductors NMR relaxation rate shows a peak below the transition temperature. The phenomenon can be explained well within the BCS weak coupling theory. In high-T_c cuprates no such peak is observed in NMR relaxation rate.

IV. Theoretical understanding – a overview

Theoretical understanding of the microscopic mechanism of pairing in high-T_c superconductors is one of the challenges of the modern theory of condensed matter physics. The high transition temperature and anomalous normal state properties of cuprates cannot be understood from a conventional theory. A number of theoretical models have been developed to describe the properties of high-T_c materials; still no common concensus has been reached on the mechanism of superconductivity. Many of the normal state properties show that the system is strongly correlated. In the following I describe in brief why a Hubbard model is considered to contain the basic physics of high-T_c systems and then a few models of superconductivity are discussed.

Anderson and his group [11] first realized that the strong correlation is playing a major role in determining the properties of high-T_c cuprate systems and a single-band Hubbard model might be the simplest hamiltonian to describe the basic physics of cuprates.

The parent material La_2CuO_4 contain one hole per Cu-ion and is an antiferromagnetic insulator. Under doping the number of holes in the CuO_2-planes increases, the AF order disappears rapidly with the increase in hole concentration and then the material becomes a superconductor in the vicinity of a metal-insulator transition.

The copper ions in the undoped material is in Cu^{2+} state having 9 electrons in the five d-orbitals. The degeneracy between the d-orbitals is removed by the crystal-field produced by the oxygen ions surrounding a Cu-ion. It can be shown that the state with highest energy has the $d_{x^2-y^2}$ character and it carries the ninth electron (or a hole). The other orbitals with lower energies are filled. In absence of any correlation the half-filled $d_{x^2-y^2}$ band should give rise to a metallic behavior. However, the undoped materials are insulators (even above the magnetic transition temperature) with long-range antiferromagnetic ordering showing that correlations are very strong. The simplest way to describe the strong correlation is to use the one-band Hubbard model, in which the strong on-site correlation U restricts the double occupancy in the system. For sufficiently large U a single-band splits into two Hubbard sub-bands separated by the Mott-Hubbard gap. It is believed that the lower Hubbard sub-band is filled whereas the upper one is empty for the undoped system (for which $n = 1$, where n is the number of electrons per site). As a result the system behaves like an insulator. Strong correlation also leads to an effective antiferromagnetic interaction through virtual hopping of electrons

between singly occupied sites in the system.

In real systems, however, the $Cu\text{-}d_{x^2-y^2}$ and $O - p_{x/y}$ bands are strongly hybridized. The additional hole, introduced by doping, go mainly to the oxygen site. This has led to a controversy whether an effective single-band model can describe the basic physics of the high-T_c systems or an explicit study of two- or three-band model is necessary. Zhang and Rice [12] argued that a hole, upon doping, resides on the square of the oxygen atoms and couples strongly to a central Cu-spin forming a local singlet. The hopping of oxygen holes now appears to be equivalent to the motion of the singlets between the respective two nearest neighbors Cu-sites. They showed that, under this situation, the hamiltonian describing charge and spin motion is the effective hamiltonian of the single-band Hubbard model in the large U limit - the so called t-J model. Schematically the antibonding band (which is mainly of d-character) splits into two Hubbard sub-bands. The non-bonding and π-bonding bands (mainly of p-character) lie in between these two Hubbard sub-bands. For the undoped system ($n = 1$) the upper Hubbard (antibonding) band is empty while the other bands with lower energies are filled. The gap to the charge excitation is then the charge transfer gap, the energy difference between the nonbonding band and the upper Hubbard band, which is much less than the Mot-Hubbard gap (energy difference between lower and upper Hubbard subbands). When additional holes are introduced by doping it goes to the nonbonding (π-bonding) band of p-character, as suggested by experiments.

The three-band model of high-T_c systems may then be mapped into an effective single-band Hubbard model where an effective Coulomb repulsion (U_{eff}) mimics the charge-transfer gap. The simplest Hubbard hamiltonian is written as

$$H = -t \sum_{ij} c_{is}^{\dagger} c_{js} + U_{eff} \sum n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

where t is the hopping integral between nearest-neighbor site and U_{eff} is the effective on-site repulsion. When $U_{eff} >> t$ and T, no doubly-occupied sites occur in the system for $n \leq 1$ and allowed hopping processes are then : (i) real hopping of holes and (ii) virtual hopping of electrons (or holes) in between two singly-occupied sites. The Hubbard hamiltonian is reduced to the $(t - J)$ model under such situation

$$H = -t \sum_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + J \sum_{ij} (S_i S_j - (1/4)\, n_i n_j) \qquad (2)$$

where $J = 4t^2/U_{eff}$. As mentioned above the first term in Eq. (1) describes motion of holes in the correlated space and second term describes the antiferromagnetic interaction induced through virtual hopping.

A. Resonating Valence Bond (RVB) Theory

For $n = 1$ the kinetic term in Eq. (2) is freezed out and the hamiltonian becomes just a spin Heisenberg hamiltonian. Anderson first suggested that for $n = 1$ the ground state of Eq. (2) for a two-dimensional square lattice is not a classical Neel state but a quantum spin liquid or resonating valence bond state. A single valence bond is a singlet state constructed from any pair of opposite spins, which need not be nearest neighbors in general. The RVB ground state corresponds to a coherent superposition of all possible configurations of valence bonds. Such a state has no long-range order (even no short-range order). An electron at a site will not show up its spin as long as its spin is paired with an opposite spin at other site, because, under this situation no site has fixed spin direction.

For the undoped material (La_2CuO_4) Anderson [11] proposed as early as 1987 that the ground state should be a RVB state. However, latter experiments reveal that the system exhibits a long-range AF order. So, the RVB state is not the lowest energy state for the undoped material. With addition of holes the AF order is destroyed very rapidly and Anderson and his coworkers [13] proposed that the RVB state is relevant in the metallic phase where there is no long-range order and the short-range order is suppressed. In the RVB background spin and charge degrees of freedom are decoupled and the quasiparticle excitations are spinons and holons. A holon carries the charge and a spinon the spin. A physical hole corresponds to a combination of a holon and a spinon. Anderson's group suggested that the resistivity in the ab-plane of cuprates is due to the scattering of holons by spinons. The density of spin excitations (spinons) grows linearly with T. So ρ_{ab} is proportional to T. For the charge conduction along the c-axis a holon and a spinon should combine to form a physical hole, which may then hop along the c-direction to the next layer. The probability of recombination of a holon and a spinon is proportional to the spinon density and thus proportional to T. So conductivity along c-

direction is proportional to T, hence $\rho_c \propto 1/T$.

The metallic behavior in the ab-plane and the semiconducting-like behavior along the c-direction may, thus, be explained within the RVB theory. However, the temperature dependence of ρ_c in high-T_c materials changes with increasing carrier density and ρ_c shows metallic behavior in the overdoped region. In fact the credibility of the RVB theory lies on the two-dimensionality of the system and dominance of the potential part (second term) in Eq. (2) than the kinetic part (first term). With increasing carrier concentration the interlayer coupling increases (as evident from the decrease of the ratio ρ_c/ρ_{ab}) and the kinetic term also becomes dominant. This restricts the applicability of the RVB theory. A RVB description is most likely to be relevant in the low-doping regime

B. Mean Field and Numerical Studies of the $t - J$ model

The exact solution of the Hubbard model is not known for more than one dimension and general filling. Mean-field results are generally useful under such situations. The basic problem in dealing Eq. (2) is to tackle the restricted hopping imposed by the strong local constraint in the correlated space. No exact method is available to treat the restrcted hopping and generally the renormalized hamiltonion mean-field approach [14-16] based on the Gutzwiller approximation [17] or the slave-boson technique [18] or the X-operator approach [19,20] is used to handle the constraint. In the renormalized hamiltonian approach (RHA) and in the mean-field slave-boson technique the local constraint is replaced by an average global constraint. The effect of correlation shows up mainly in the effective mass, otherwise the system behaves as an uncorrelated one. In the X-operator technique, on the other hand, the local constraint is imposed rather strictly. The potential energy part in the t-J model (second term in Eq. 2) leads to interactions between quasiparticles which, in mean-filed theory, result in a superconducting ground state with extended singlet pairing. Many authors [14-16,18-22] have studied superconductivity in the t-J and t-J-v models within the mean-field theories

$$H = -t \sum_{i,j} c^{\dagger}_{i,s} c_{j,s} + J \sum_{i,j} (S_i S_j - (1/4)\, n_i n_j) - v \sum_{i,j} n_i n_j \qquad (3)$$

where v is an additional intersite attractive interaction between charge carriers. In general, it may arise through the polarization of a bosonic field in the vicinity of the charge carrier when a linear coupling between the bosonic filed

and the electron number operator exists. The bosonic field may be phonons, excitons, acoustic plasmons, magnons, etc. The interaction v acts as an additional channel for superconductivity.

The t-J and the t-J-v models have been studied extensively within the RHA [14-16,21] and the X-operator technique [19,20,22]. The RHA predicts d-wave superconductivity for a wide range of hole concentrations starting from zero hole concentration ($x = 1 - n = 0$), and extended s-wave for low-electron concentrations ($n \sim 0$). At $x = 0$, the RHA predicts a high value of the transition temperature which is an artifact of the approximation.

The X-operator technique predicts extended s-wave superconductivity for low-hole concentrations ($x \sim 0$) as well as for low-electron concentrations ($n \sim 0$) and d-wave pairing for a wide range of intermediate hole concentrations.

The X-operator predictions for superconducting phase diagram and normal state properties are much more consistent with the experimental results of high-T_c oxide systems than that predicted by the RHA [19,20].

Finite size clusters of the t-J model have been analyzed extensively by exact diagonalization and variational Monte Carlo technique. These studies indicate that several of the anomalous normal state properties of the cuprate superconductors could be accounted for by the t-J model. Recent numerical studies [23] for the superconducting correlations predict a d-wave superconductivity for a wide range of electron concentrations and a transition to s-wave superconductivity is observed on decreasing the electronic density ($n < 0.2$). Near half-filling ($n \sim 1$) no robust signals of a superconducting phase is obtained. In fact, for low-hole concentrations it is very difficult to identify a superconducting ground state using finite clusters because a few number of pairs are available [23].

C. van Hove Singularity Scenario

Correlation induced mechanism or any electronic mechanism cannot account for the isotope effect in high-T_c systems. Large values of the isotope-shift exponent (α) have been observed in some superconducting samples at proper doping [9]. This suggests that phonons are also playing an important role in the mechanism of high-T_c superconductivity. Many workers [24,25] have been studying the van Hove scenario, which is based on the BCS phonon-mediated pairing, to explain the anomalous properties of high-T_c systems. It is known

that presence of a van Hove singularity (VHS) in the density of states (DOS) enhances the BCS transition temperature when the Fermi level is at or near the VHS point. A two-dimensional system has at least one VHS in the DOS. The credibility of the VHS scenario lies on the quasi two-dimensional structure of the cuprates and the observation that the Fermi level is in the vicinity of the VHS point of the DOS for optimum doping (at which T_c is maximum). Tsuei *et al.* [24] first pointed out that the anomalous isotope effect in La-214 system may be qualitatively explained within the VHS scenario. Sarkar and Das [25] studied the isotope-shift exponent, pressure coefficient of T_c and the superconducting gap to T_c ratio exactly within the VHS scenario. α and the pressure coefficient of T_c show low values (minimum for α) at optimum doping and larger values for underdoped systems. The behavior agrees qualitatively with experimental results. However, α_{min} is found to be much larger than that observed experimentally. The gap to T_c ratio is close to the BCS value. So only a VHS in the DOS cannot explain the properties of high-T_c systems.

D. Interlayer Pair Tunneling Mechanism

Anderson and his group [11,13,26] proposed that in high-T_c cuprate superconductors, which are described by the 2-D t-J model, the charge and the spin degrees of freedom are decoupled. Because of charge-spin decoupling single electron hopping between two CuO_2 planes is suppressed. However, the second-order processes in interlayer hopping do not leave any unpaired spin in a layer and are not suppressed. In the language of spinons and holons the interplane coupling causes pairs of holons to hop between layer by creating or annihilating spinon pairs. It should be remembered that a pair of holons is equivalent to a pair of (real) holes in the singlet state. Anderson has proposed that this interlayer pair tunneling term is responsible for the high transition temperature in oxide superconductors. Recent numerical study [27] shows that the superconducting correlation is enhanced by the interlayer coupling term.

Chakravarty *et al.* [28] studied the interlayer tunneling mechanism and found that this mechanism can lead to a high transition temperature, an anisotropic s-wave superconducting gap and an absence of Hebel-Slichter peak in the NMR relaxation rate, as observed in experiments. They assumed that the electron-phonon (e-ph) interaction is the dominant mechanism for in-plane pairing in order to explain anomalous isotope effect observed in high-T_c systems. The interlayer pair tunneling enhances the pairing mechanism by allow-

ing the Cooper pairs (formed due to e-ph interactions in the plane) to tunnel to an adjacent layer provided coherent interlayer single particle hopping is blocked. However, the fact that ρ_c shows metallic behavior for good metallic superconducting samples poses a serious question to the interlayer pair tunneling mechanism which stands solely on the assumption that the single particle hopping is blocked. For Y-123 compound at optimum doping T_c is not affected by the pressure along the c-axis; this does not comply with the interlayer pair tunneling mechanism.

V. Final Remarks

All high-Tc cuprate oxide systems have common characteristic properties. Different models have been proposed for the mechanism of the superconductivity and anomalous normal state properties of the cuprates. Major groups share the view that the strong correlation is playing an important role for the anomalous properties of cuprates. There are other groups who have not incorporated strong correlation in their theories. It is not possible to cover all the theories in this article which is based on a single talk. Polaronic theory, spin-bag theory, spin-fluctuation mechanism etc. are not at all addressed in this article. Large numbers of published papers on different models clearly show that the origin of superconductivity in cuprates is yet to understand. However analysis of the experimental results indicates (at least to the author) that the model based on strong correlation and e-ph interaction is a potential candidate for describing the high-T_c cuprate systems.

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